## Supplementary data for

## A novel drug-drug cocrystal of tegafur and myricetin: optimized properties of dissolution and tabletability

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Fig. S1 PXRD patterns for MYR·H<sub>2</sub>O after heating to 280 or 320 °C and cooling to room temperature in the DSC test.



Fig. S2 <sup>1</sup>H-NMR spectra of TGF-MYR with integrals.



Fig. S3 PXRD patterns of TGF, MYR·H<sub>2</sub>O and TGF-MYR after dissolution test at pH 6.8.



Fig. S4 The 2D waved structure of TGF.



Fig. S5 PXRD patterns of TGF, MYR·H<sub>2</sub>O and TGF-MYR after compaction experiments at 300 MPa.





Fig. S6 PXRD patterns for (a) TGF and TGF-MYR, and (b) MYR·H<sub>2</sub>O involved in DVS tests.





Fig. S7 PXRD patterns of (a) TGF, (b) MYR·H<sub>2</sub>O and (c) TGF-MYR during storage under 40 °C /75% RH.